

```
chain nodes :
    14 15
            16
                17
                    18
                        19
                            20
                                    22
                                                29
                                21
                                        23
                                            28
                                                    30
                                                        32
                                                            33
                                                                34
                                                                     37
                                                                         38
                                                                             39
                                                                                42
        47
                    50
                        51
    46
                                                57
           48
                49
                            52
                                53
                                    54
                                        55
                                            56
                                                    58
                                                        59
                                                            60
                                                                61
                                                                    62
                                                                        63
                                                                             64
                                                                                 65
                                                                                     66
                                                                                         75
ring nodes :
    1 2 3
               5 6 7
                         8
                            9
                               10
                                   11 12
chain bonds:
         5-38 11-37 14-17 15-16 16-18 19-20 21-22 21-23 28-29 28-30 32-33 32-34
          39-42 39-44 39-75 45-46 46-47 48-49 48-50 51-52 52-53 52-54 55-56 56-57
    38-39
    56-58 59-60 61-62 63-64 64-65 64-66
ring bonds :
    1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12
exact/norm bonds :
    2-37 5-38 11-37 28-29 28-30 32-33 32-34 38-39 39-44 39-75 45-46 46-47 48-49 48-50 51-52 52-53 52-54 55-56 56-57 56-58 59-60 61-62 63-64 64-65 64-66
exact bonds :
    14-17 15-16 16-18 19-20 21-22 21-23 39-42
normalized bonds:
    1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12
isolated ring systems :
    containing 1:7:
G1:[*1],[*2],[*3],[*4],[*5],[*6]
G2:H,CH3,Et
G3:[*5],[*6],[*7],[*8],[*9],[*10],[*11],[*12],[*13]
Match level :
    1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom
    12:Atom 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS 19:CLASS 20:CLASS 21:CLASS
```

30:CLASS

45:CLASS

54:CLASS

32:CLASS

46:CLASS

55:CLASS

33:CLASS

47:CLASS

56:CLASS

34:CLASS

48:CLASS

57:CLASS

37:CLASS

49:CLASS

58:CLASS

29:CLASS

44:CLASS

53:CLASS

22:CLASS

38:CLASS

50:CLASS

59:CLASS

23:CLASS

39:CLASS

51:CLASS

28:CLASS

42:CLASS

52:CLASS

```
C:\stnweb\Queries\3.str
chain nodes :
```

```
14 15
              17
          16
                  18
                      19
                          20
                                        28
                                                       33
                                                                          42
                                                                             44
                                                                                 45
    46 47 48
              49 50 51
                             53
                                 54
                                    55
                                            57
                                                    59
                          52
                                                58
                                        56
                                                       60
                                                           61
                                                              62
                                                                  63
                                                                      64
                                                                          65
                                                                             66
                                                                                 75
ring nodes :
    1 2 3
                      8
                         9
                            10
                                11
                                   12
chain bonds:
    2-37 5-38 12-37 14-17 15-16 16-18 19-20 21-22 21-23 28-29 28-30 32-33 32-34
    38-39 39-42 39-44 39-75 45-46 46-47 48-49 48-50 51-52 52-53 52-54 55-56 56-57
    56-58 59-60 61-62 63-64 64-65 64-66
ring bonds :
   1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12
exact/norm bonds :
   2-37 5-38 12-37 28-29 28-30 32-33 32-34 38-39 39-44 39-75 45-46 46-47 48-49
   48-50 51-52 52-53 52-54 55-56 56-57 56-58 59-60 61-62 63-64 64-65 64-66
exact bonds
   14-17 15-16 16-18 19-20 21-22 21-23
                                         39-42
normalized bonds:
   1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12
isolated ring systems :
   containing 1 : 7 :
G1:[*1],[*2],[*3],[*4],[*5],[*6]
G2:H,CH3,Et
```

Match level: 1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom 16:CLASS 17:CLASS 18:CLASS 19:CLASS 20:CLASS 21:CLASS 12:Atom 14:CLASS 15:CLASS 22:CLASS 23:CLASS 28:CLASS 29:CLASS 30:CLASS 32:CLASS 33:CLASS 34:CLASS 37:CLASS 39:CLASS 44:CLASS 38:CLASS 42:CLASS 45:CLASS 47:CLASS 46:CLASS 48:CLASS 49:CLASS 50:CLASS 51:CLASS 52:CLASS 53:CLASS 54:CLASS 55:CLASS 56:CLASS 57:CLASS 58:CLASS 59:CLASS

G3: [*5], [*6], [*7], [*8], [*9], [*10], [*11], [*12], [*13]

```
C:\stnweb\queries\5b.str
```

```
chain nodes :
   14 15 16
46 47 48
               17
                  18
                      19
                          20
                                  22
                                     23
                              21
                                         28
                                             29
                                                 30
                                                    32
                                                        33
                                                            34
                                                                37
                                                                    38
                                                                       39
                                                                           42
                                                                              44
              49 50
                     51
                          52
                              53
                                             57
                                  54
                                     55
                                         56
                                                 58
                                                     59
                                                        60
                                                            61
                                                                62
                                                                    63
                                                                       64
ring nodes :
    1 2 3
               5 6 7
                       8
                          9
                             10
                                11
                                    12
chain bonds :
    2-37 5-38 7-37 14-17 15-16 16-18 19-20 21-22 21-23 28-29 28-30 32-33 32-34
          39-42 39-44 39-75 45-46 46-47 48-49 48-50 51-52 52-53 52-54 55-56 56-57
    38-39
    56-58 59-60 61-62 63-64 64-65
                                    64-66
ring bonds :
    1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12
exact/norm bonds :
   2-37 5-38 7-37 28-29 28-30 32-33 32-34 38-39 39-44 39-75 45-46 46-47 48-49
          51-52 52-53 52-54 55-56 56-57 56-58 59-60 61-62 63-64 64-65 64-66
    48-50
exact bonds
   14-17 15-16 16-18 19-20 21-22 21-23 39-42
normalized bonds:
   1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12
isolated ring systems :
   containing 1 : 7 :
G1:[*1],[*2],[*3],[*4],[*5],[*6]
G2:H,CH3,Et
G3:[*5],[*6],[*7],[*8],[*9],[*10],[*11],[*12],[*13]
Match level:
```

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom 12:Atom 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS 19:CLASS 20:CLASS 21:CLASS

30:CLASS

45:CLASS

54:CLASS

32:CLASS

46:CLASS

55:CLASS

33:CLASS

47:CLASS

56:CLASS

34:CLASS

48:CLASS

57:CLASS

37:CLASS

49:CLASS

58:CLASS

22:CLASS

38:CLASS

50:CLASS

59:CLASS

23:CLASS

39:CLASS

51:CLASS

28:CLASS

42:CLASS

52:CLASS

29:CLASS

44:CLASS

53:CLASS

=> file reg COST IN U.S. DOLLARS

SINCE FILE TOTAL
ENTRY SESSION
2.48 166.93

FULL ESTIMATED COST

FILE 'REGISTRY' ENTERED AT 11:53:58 ON 12 AUG 2004
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2004 American Chemical Society (ACS)

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 11 AUG 2004 HIGHEST RN 725685-10-9 DICTIONARY FILE UPDATES: 11 AUG 2004 HIGHEST RN 725685-10-9

TSCA INFORMATION NOW CURRENT THROUGH MAY 21, 2004

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at: http://www.cas.org/ONLINE/DBSS/registryss.html

=> L5

STRUCTURE UPLOADED

=> d 1.5

L5 HAS NO ANSWERS

L5 STR

=> s 15

SAMPLE SEARCH INITIATED 11:55:47 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 44 TO ITERATE

100.0% PROCESSED 44 ITERATIONS

0 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS:

483 TO 1277

PROJECTED ANSWERS:

0 TO

L6 0 SEA SSS SAM L5

=> s 15 full

THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 155.00 U.S. DOLLARS DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END: Y FULL SEARCH INITIATED 11:55:51 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 927 TO ITERATE

100.0% PROCESSED 927 ITERATIONS

0 ANSWERS

SEARCH TIME: 00.00.01

L7 0 SEA SSS FUL L5

=>

STRUCTURE UPLOADED L8

=> d 19

L8 HAS NO ANSWERS

=> s 18

SAMPLE SEARCH INITIATED 11:56:41 FILE 'REGISTRY' SAMPLE SCREEN SEARCH COMPLETED - 43 TO ITERATE

100.0% PROCESSED 43 ITERATIONS

0 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS:

467 TO 1253

PROJECTED ANSWERS:

O TO

T.9 0 SEA SSS SAM L8

=> s 18 full

THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 155.00 U.S. DOLLARS DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y FULL SEARCH INITIATED 11:56:45 FILE 'REGISTRY' FULL SCREEN SEARCH COMPLETED - 759 TO ITERATE

100.0% PROCESSED 759 ITERATIONS

O ANSWERS

SEARCH TIME: 00.00.01

O SEA SSS FUL L8 L10

=>

L11 STRUCTURE UPLOADED

=> d 111

L11 HAS NO ANSWERS

L11

STR

=> s 111

SAMPLE SEARCH INITIATED 11:57:41 FILE 'REGISTRY' SAMPLE SCREEN SEARCH COMPLETED - 44 TO ITERATE

100.0% PROCESSED 44 ITERATIONS

0 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS:

483 TO 1277

PROJECTED ANSWERS:

0 TO , 0

0 SEA SSS SAM L11

=> s lll full

THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 155.00 U.S. DOLLARS DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y FULL SEARCH INITIATED 11:57:46 FILE 'REGISTRY' FULL SCREEN SEARCH COMPLETED - 1024 TO ITERATE

100.0% PROCESSED 1024 ITERATIONS

0 ANSWERS

eb

SEARCH TIME: 00.00.01

L13

0 SEA SSS FUL L11

=> log y COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

467.94

634.87

STN INTERNATIONAL LOGOFF AT 11:58:11 ON 12 AUG 2004